Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:02 AM GMT

PDB ID	:	2FCP
Title	:	FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI
Authors	:	Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.
Deposited on	:	1998-10-15
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

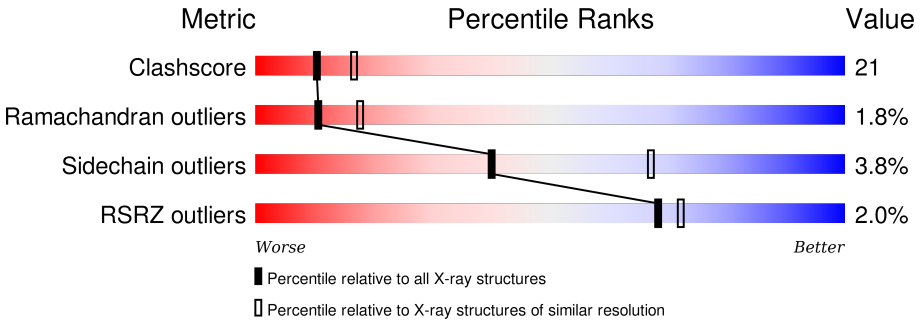
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	2% 62% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	A	1006	-	-	X	-
3	GLA	A	1009	-	-	X	-
6	LIL	A	903	-	-	-	X
6	LIL	A	904	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	LIM	A	906	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5512	3469	942	1087	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	INSERTION	UNP P06971
A	407	HIS	-	INSERTION	UNP P06971
A	408	HIS	-	INSERTION	UNP P06971
A	409	HIS	-	INSERTION	UNP P06971
A	410	HIS	-	INSERTION	UNP P06971
A	411	HIS	-	INSERTION	UNP P06971
A	412	HIS	-	INSERTION	UNP P06971
A	413	GLY	-	INSERTION	UNP P06971
A	414	SER	-	INSERTION	UNP P06971

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	5	Total	C	N	O	P	0	0
			74	35	2	35	2		

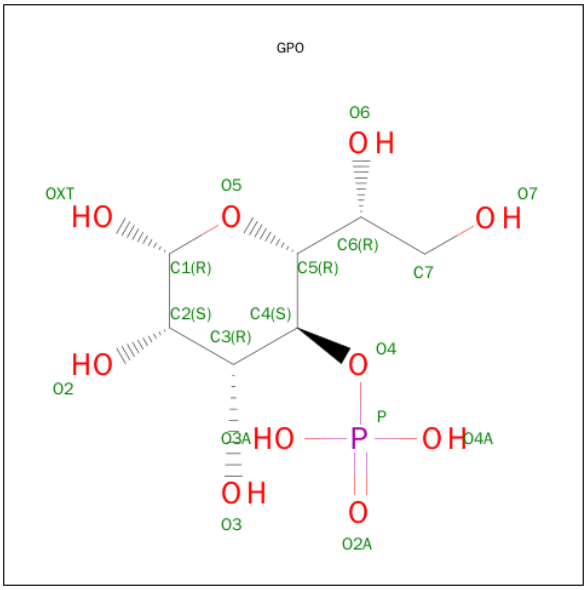
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	3	Total	C	O	0	0
			33	18	15		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

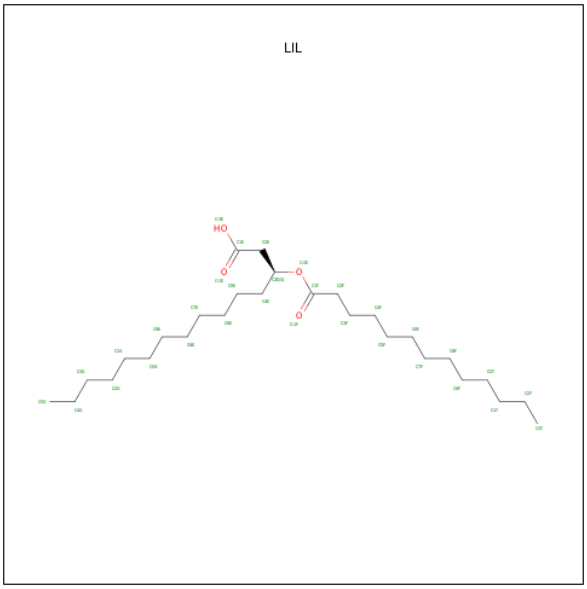
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ni 2 2	0	0

- Molecule 5 is 4-O-PHOSPHONO-D-GLYCERO-BETA-D-MANNO-HEPTOPYRANOSE (three-letter code: GPO) (formula: $C_7H_{15}O_{10}P$).



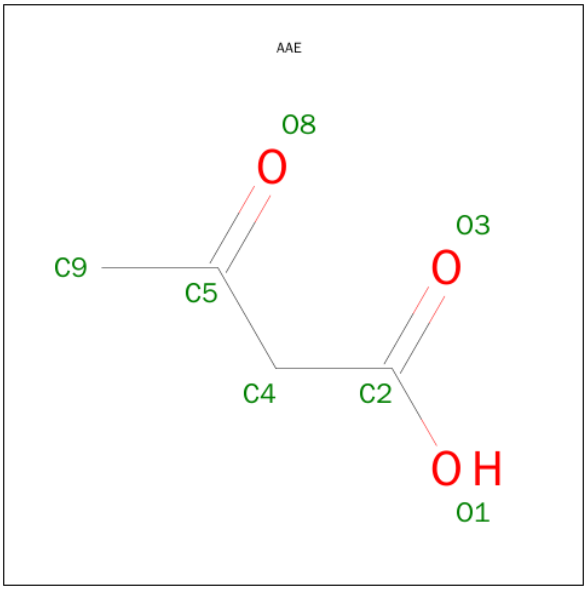
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O P 17 7 9 1	0	0

- Molecule 6 is 2-TRIDECANOYLOXY-PENTADECANOIC ACID (three-letter code: LIL) (formula: $C_{28}H_{54}O_4$).



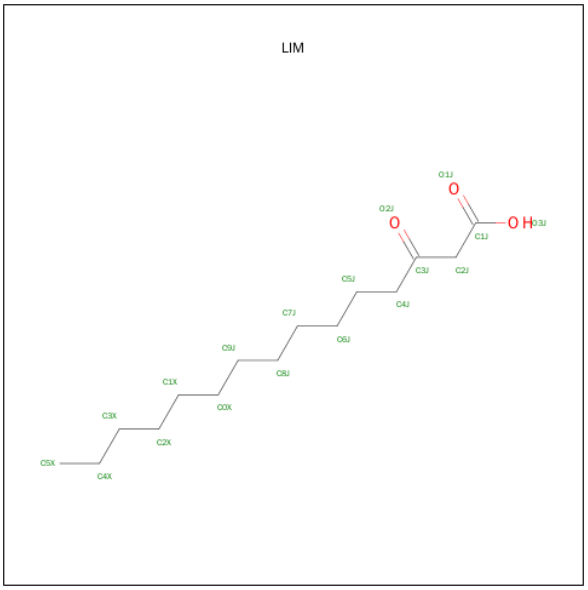
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 31 28 3	0	0
6	A	1	Total C O 31 28 3	0	0

- Molecule 7 is ACETOACETIC ACID (three-letter code: AAE) (formula: $C_4H_6O_3$).



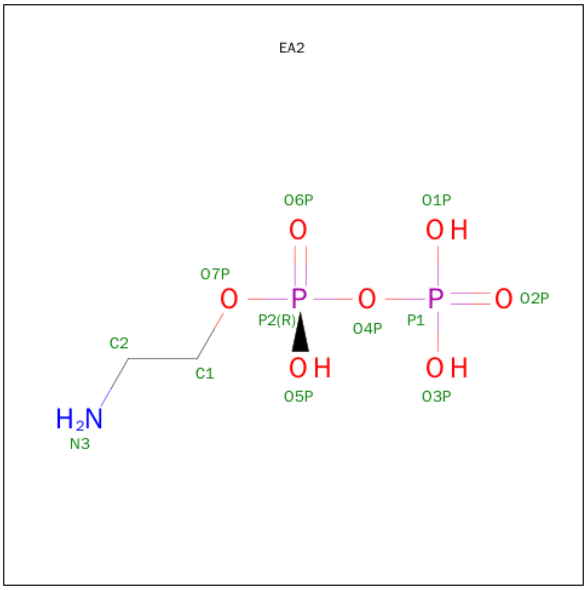
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 4 2	0	0

- Molecule 8 is 3-OXO-PENTADECANOIC ACID (three-letter code: LIM) (formula: $C_{15}H_{28}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 17 15 2	0	0

- Molecule 9 is AMINOETHANOLPYROPHOSPHATE (three-letter code: EA2) (formula: $C_2H_9NO_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O P 11 2 1 6 2	0	0

- Molecule 10 is water.

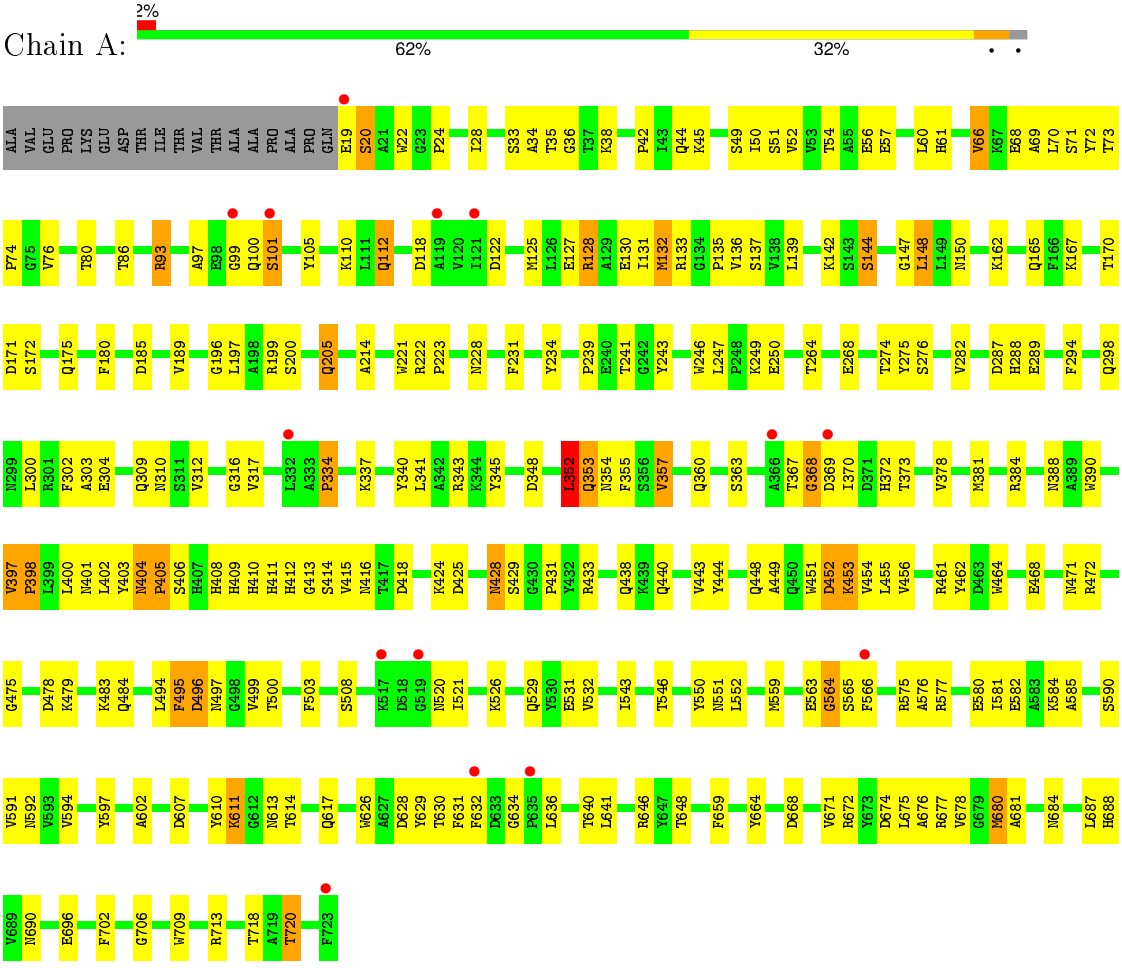
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	99	Total O 99 99	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	171.55Å 171.55Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 43.12 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.50) 98.8 (43.12-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.45Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.242 , 0.283 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.0	EDS
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 53749 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5833	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AAE, NI, GMH, LIL, GLA, GLC, KDO, GPO, LIM, GP4, EA2, GP1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/5652	0.66	1/7680 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5512	0	5213	221	0
2	A	74	0	46	3	0
3	A	33	0	28	6	0
4	A	2	0	0	0	0
5	A	17	0	10	0	0
6	A	62	0	106	14	0
7	A	6	0	5	1	0
8	A	17	0	27	5	0
9	A	11	0	6	1	0
10	A	99	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5833	0	5441	240	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:HG23	1:A:241:THR:HG21	1.35	1.04
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.32	1.04
1:A:132:MET:HG2	1:A:136:VAL:HG11	1.50	0.93
1:A:408:HIS:O	1:A:411:HIS:HB3	1.69	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.57	0.83
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.46	0.80
3:A:1006:GLC:C6	3:A:1009:GLA:H5	2.12	0.79
1:A:341:LEU:HB2	1:A:402:LEU:HD11	1.62	0.79
1:A:468:GLU:HG3	1:A:479:LYS:HG2	1.66	0.78
1:A:378:VAL:HG12	1:A:443:VAL:HG12	1.65	0.77
1:A:19:GLU:HG3	1:A:632:PHE:CE2	2.20	0.76
3:A:1006:GLC:H62	3:A:1009:GLA:H5	1.66	0.75
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.53	0.72
1:A:35:THR:HG22	1:A:150:ASN:HD22	1.57	0.70
1:A:713:ARG:HG2	1:A:713:ARG:HH11	1.56	0.70
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.28	0.68
6:A:904:LIL:H9F1	8:A:906:LIM:H5X2	1.75	0.68
1:A:565:SER:O	1:A:566:PHE:HB2	1.92	0.67
1:A:343:ARG:HH11	1:A:400:LEU:HG	1.58	0.67
1:A:298:GLN:HE22	8:A:906:LIM:H3X1	1.59	0.67
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.30	0.67
1:A:668:ASP:OD1	1:A:690:ASN:HA	1.95	0.66
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.08	0.66
1:A:671:VAL:HG22	1:A:687:LEU:HB3	1.78	0.66
1:A:189:VAL:HG23	1:A:222:ARG:O	1.95	0.65
1:A:352:LEU:HB2	1:A:384:ARG:O	1.95	0.65
1:A:135:PRO:HB3	1:A:508:SER:HB3	1.79	0.64
1:A:353:GLN:HG3	10:A:1039:HOH:O	1.98	0.64
1:A:408:HIS:O	1:A:411:HIS:CB	2.45	0.63
3:A:1006:GLC:C6	3:A:1009:GLA:C5	2.77	0.63
1:A:428:ASN:HD22	1:A:429:SER:N	1.95	0.63
1:A:592:ASN:HB2	1:A:628:ASP:OD1	1.99	0.63
1:A:626:TRP:CH2	1:A:628:ASP:HB3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:HB2	1:A:44:GLN:NE2	2.13	0.63
1:A:584:LYS:HG2	1:A:594:VAL:HG13	1.81	0.62
1:A:390:TRP:CE2	1:A:424:LYS:HB3	2.34	0.62
1:A:677:ARG:NH1	1:A:677:ARG:HB3	2.15	0.62
1:A:610:TYR:O	1:A:611:LYS:HB2	1.98	0.62
1:A:428:ASN:C	1:A:428:ASN:HD22	2.03	0.61
3:A:1006:GLC:H61	3:A:1009:GLA:H3	1.82	0.61
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.82	0.61
1:A:675:LEU:HB2	1:A:684:ASN:HA	1.82	0.61
1:A:412:HIS:CD2	1:A:413:GLY:H	2.20	0.60
1:A:35:THR:HG23	1:A:130:GLU:OE1	2.01	0.60
1:A:702:PHE:CE2	1:A:706:GLY:HA3	2.37	0.60
1:A:71:SER:HB3	1:A:646:ARG:HD3	1.82	0.60
1:A:343:ARG:O	1:A:397:VAL:HG13	2.02	0.60
1:A:401:ASN:OD1	1:A:403:TYR:HB2	2.02	0.60
1:A:676:ALA:CB	1:A:681:ALA:HA	2.32	0.59
1:A:671:VAL:CG2	1:A:687:LEU:HB3	2.32	0.59
1:A:72:TYR:CE2	1:A:626:TRP:HB2	2.37	0.59
1:A:148:LEU:HD23	1:A:148:LEU:C	2.23	0.59
1:A:444:TYR:HB3	1:A:461:ARG:HB2	1.84	0.59
1:A:42:PRO:HB2	1:A:44:GLN:HE22	1.68	0.59
6:A:903:LIL:H9E2	6:A:904:LIL:H0S1	1.84	0.58
1:A:384:ARG:HD3	10:A:1039:HOH:O	2.03	0.58
1:A:294:PHE:HE1	1:A:363:SER:HG	1.52	0.57
1:A:529:GLN:HB2	1:A:552:LEU:HD13	1.85	0.57
1:A:132:MET:HG2	1:A:136:VAL:CG1	2.30	0.57
1:A:343:ARG:NH1	1:A:400:LEU:HG	2.20	0.57
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.39	0.57
1:A:51:SER:OG	1:A:133:ARG:NH2	2.37	0.57
1:A:453:LYS:HE2	1:A:453:LYS:N	2.20	0.57
1:A:300:LEU:C	1:A:300:LEU:HD23	2.25	0.57
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.35	0.56
1:A:264:THR:HA	1:A:709:TRP:CD1	2.40	0.56
1:A:409:HIS:O	1:A:412:HIS:O	2.23	0.56
1:A:73:THR:HG22	10:A:1032:HOH:O	2.05	0.56
1:A:142:LYS:HG2	1:A:440:GLN:OE1	2.05	0.56
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.06	0.55
1:A:97:ALA:HB3	1:A:101:SER:O	2.06	0.55
1:A:132:MET:CG	1:A:136:VAL:HG11	2.30	0.55
1:A:36:GLY:HA2	1:A:132:MET:SD	2.46	0.55
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH2	1:A:531:GLU:OE1	2.30	0.55
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.88	0.54
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.88	0.54
1:A:590:SER:O	1:A:629:TYR:HA	2.07	0.54
1:A:24:PRO:O	1:A:28:ILE:HG12	2.08	0.54
1:A:676:ALA:HB2	1:A:681:ALA:HA	1.90	0.54
1:A:449:ALA:HB3	1:A:456:VAL:CG1	2.38	0.54
1:A:676:ALA:HA	1:A:680:MET:O	2.08	0.54
1:A:415:VAL:HG22	1:A:416:ASN:N	2.23	0.54
1:A:543:ILE:HG22	1:A:585:ALA:HB1	1.90	0.54
1:A:373:THR:HB	1:A:448:GLN:HB2	1.89	0.53
3:A:1006:GLC:H62	3:A:1009:GLA:C5	2.35	0.53
1:A:404:ASN:HB2	10:A:1046:HOH:O	2.07	0.53
1:A:54:THR:OG1	1:A:57:GLU:HG3	2.08	0.53
3:A:1006:GLC:H61	3:A:1009:GLA:H5	1.88	0.53
1:A:70:LEU:HD22	1:A:131:ILE:HG13	1.90	0.53
1:A:453:LYS:HE2	1:A:453:LYS:H	1.72	0.53
1:A:591:VAL:HG22	1:A:629:TYR:HD1	1.73	0.53
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.44	0.53
1:A:302:PHE:CZ	6:A:903:LIL:H2E1	2.44	0.52
1:A:334:PRO:HA	1:A:337:LYS:HE2	1.91	0.52
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.44	0.52
1:A:713:ARG:NH1	1:A:713:ARG:HG2	2.24	0.52
1:A:381:MET:HE3	10:A:1022:HOH:O	2.09	0.52
1:A:353:GLN:CG	10:A:1039:HOH:O	2.58	0.52
1:A:93:ARG:HG3	1:A:550:TYR:OH	2.10	0.52
6:A:904:LIL:H7F1	8:A:906:LIM:H0X2	1.92	0.51
1:A:110:LYS:HD3	1:A:112:GLN:HG2	1.92	0.51
1:A:546:THR:HG22	1:A:582:GLU:HB3	1.92	0.51
1:A:228:ASN:HB3	1:A:287:ASP:OD1	2.11	0.51
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.92	0.51
2:A:1004:GMH:H6	9:A:1008:EA2:O6P	2.10	0.51
1:A:575:ARG:CZ	1:A:577:ARG:HE	2.23	0.51
1:A:406:SER:O	1:A:410:HIS:HD2	1.94	0.51
1:A:93:ARG:HH11	1:A:580:GLU:CD	2.13	0.51
1:A:602:ALA:O	1:A:614:THR:HG22	2.10	0.51
1:A:264:THR:HG21	1:A:696:GLU:HG2	1.92	0.51
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.76	0.51
1:A:671:VAL:HG23	1:A:671:VAL:O	2.11	0.51
1:A:132:MET:O	1:A:147:GLY:HA2	2.11	0.50
1:A:370:ILE:HG12	1:A:451:TRP:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TRP:CZ2	1:A:424:LYS:HB2	2.46	0.50
1:A:449:ALA:HB3	1:A:456:VAL:HG13	1.93	0.50
1:A:370:ILE:HG12	1:A:451:TRP:HD1	1.76	0.50
1:A:390:TRP:HE1	1:A:429:SER:CB	2.23	0.50
1:A:404:ASN:O	1:A:406:SER:N	2.45	0.50
1:A:640:THR:HB	1:A:672:ARG:HB3	1.94	0.50
1:A:73:THR:CG2	10:A:1032:HOH:O	2.60	0.49
1:A:19:GLU:O	1:A:20:SER:HB3	2.12	0.49
1:A:367:THR:HG22	1:A:367:THR:O	2.13	0.49
1:A:35:THR:HG22	1:A:150:ASN:ND2	2.28	0.49
1:A:196:GLY:HA2	1:A:214:ALA:O	2.13	0.49
1:A:60:LEU:HD21	1:A:626:TRP:HH2	1.76	0.49
6:A:903:LIL:C9F	6:A:903:LIL:H2S1	2.43	0.49
1:A:626:TRP:NE1	10:A:1020:HOH:O	2.34	0.48
1:A:282:VAL:HG21	6:A:903:LIL:C9E	2.44	0.48
1:A:298:GLN:NE2	8:A:906:LIM:H3X1	2.26	0.48
1:A:388:ASN:HD22	1:A:433:ARG:HG2	1.77	0.48
1:A:142:LYS:O	1:A:142:LYS:HG3	2.12	0.48
1:A:68:GLU:OE1	1:A:68:GLU:N	2.36	0.48
1:A:368:GLY:O	1:A:369:ASP:HB2	2.14	0.48
1:A:495:PHE:HB2	1:A:499:VAL:O	2.14	0.48
1:A:170:THR:HG22	1:A:171:ASP:H	1.78	0.47
1:A:38:LYS:HD3	1:A:360:GLN:HE22	1.79	0.47
1:A:559:MET:SD	1:A:607:ASP:HA	2.54	0.47
1:A:231:PHE:CZ	6:A:903:LIL:H4S2	2.48	0.47
1:A:453:LYS:HE2	1:A:453:LYS:CA	2.43	0.47
1:A:440:GLN:HA	1:A:464:TRP:O	2.13	0.47
1:A:19:GLU:HG3	1:A:632:PHE:CZ	2.48	0.47
1:A:462:TYR:OH	1:A:483:LYS:HB3	2.14	0.47
1:A:316:GLY:O	1:A:341:LEU:HD12	2.15	0.47
1:A:345:TYR:CD1	1:A:345:TYR:C	2.88	0.47
1:A:641:LEU:CD2	1:A:671:VAL:HG12	2.45	0.47
1:A:390:TRP:CZ3	1:A:431:PRO:HG3	2.50	0.47
1:A:590:SER:HB2	1:A:630:THR:O	2.15	0.47
1:A:165:GLN:HG3	1:A:720:THR:HB	1.97	0.47
1:A:93:ARG:HG3	1:A:550:TYR:CZ	2.49	0.47
1:A:142:LYS:NZ	1:A:438:GLN:OE1	2.48	0.46
1:A:246:TRP:O	1:A:247:LEU:HD23	2.15	0.46
1:A:50:ILE:HB	1:A:132:MET:CE	2.44	0.46
1:A:45:LYS:HB3	1:A:455:LEU:CD2	2.45	0.46
1:A:304:GLU:HA	1:A:352:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:903:LIL:H2S1	6:A:903:LIL:H9F2	1.98	0.46
1:A:412:HIS:CG	1:A:413:GLY:N	2.84	0.46
1:A:648:THR:HB	1:A:664:TYR:CE1	2.50	0.46
1:A:60:LEU:HD21	1:A:626:TRP:CH2	2.50	0.46
1:A:413:GLY:O	1:A:414:SER:HB2	2.15	0.46
1:A:137:SER:HB2	1:A:508:SER:HA	1.96	0.46
1:A:520:ASN:ND2	10:A:1101:HOH:O	2.49	0.46
1:A:303:ALA:O	1:A:353:GLN:HA	2.16	0.46
1:A:93:ARG:NH1	1:A:580:GLU:OE1	2.48	0.46
6:A:903:LIL:H8E1	6:A:904:LIL:H8E1	1.97	0.45
1:A:425:ASP:HB3	1:A:428:ASN:ND2	2.32	0.45
2:A:902:GP1:O4B	7:A:905:AAE:O3	2.27	0.45
1:A:282:VAL:HG21	6:A:903:LIL:H9E1	1.99	0.45
1:A:22:TRP:CD1	1:A:60:LEU:HD22	2.52	0.45
1:A:563:GLU:O	1:A:564:GLY:C	2.56	0.45
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.37	0.45
1:A:170:THR:HG22	1:A:171:ASP:N	2.31	0.45
1:A:61:HIS:HD2	10:A:1110:HOH:O	2.00	0.45
1:A:288:HIS:HD2	1:A:289:GLU:N	2.15	0.44
1:A:199:ARG:HD2	10:A:1093:HOH:O	2.16	0.44
1:A:197:LEU:HD12	1:A:197:LEU:C	2.38	0.44
1:A:629:TYR:HE2	1:A:631:PHE:CE1	2.35	0.44
1:A:137:SER:CB	1:A:508:SER:HA	2.47	0.44
1:A:415:VAL:HG22	1:A:416:ASN:H	1.81	0.44
1:A:99:GLY:O	1:A:100:GLN:HB2	2.17	0.44
1:A:51:SER:OG	1:A:73:THR:HG23	2.17	0.44
1:A:80:THR:CG2	1:A:617:GLN:NE2	2.80	0.44
1:A:678:VAL:O	1:A:678:VAL:HG12	2.18	0.44
1:A:60:LEU:O	1:A:688:HIS:HE1	2.01	0.43
1:A:575:ARG:HG2	1:A:576:ALA:N	2.33	0.43
1:A:171:ASP:O	1:A:172:SER:HB2	2.18	0.43
1:A:137:SER:OG	1:A:508:SER:HA	2.19	0.43
1:A:50:ILE:HB	1:A:132:MET:HE3	2.01	0.43
1:A:52:VAL:HG22	1:A:130:GLU:HG2	2.00	0.43
1:A:452:ASP:C	1:A:454:VAL:H	2.21	0.43
1:A:484:GLN:OE1	1:A:526:LYS:HE2	2.19	0.43
1:A:690:ASN:O	1:A:713:ARG:HA	2.17	0.43
1:A:631:PHE:HB2	1:A:636:LEU:O	2.19	0.43
1:A:247:LEU:HD21	1:A:268:GLU:HG3	2.00	0.43
1:A:49:SER:HB3	1:A:133:ARG:NH1	2.33	0.43
1:A:355:PHE:CE2	1:A:357:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:HA	1:A:144:SER:HB2	2.00	0.43
1:A:456:VAL:O	1:A:456:VAL:HG13	2.18	0.43
1:A:309:GLN:HG2	1:A:348:ASP:HB3	2.00	0.43
1:A:409:HIS:C	1:A:411:HIS:H	2.21	0.43
1:A:390:TRP:CE2	1:A:424:LYS:CB	3.02	0.42
1:A:66:VAL:O	1:A:69:ALA:HB3	2.19	0.42
1:A:402:LEU:C	1:A:405:PRO:HD2	2.39	0.42
1:A:646:ARG:HG3	1:A:646:ARG:HH11	1.84	0.42
1:A:249:LYS:HD2	1:A:659:PHE:CD2	2.55	0.42
1:A:478:ASP:HB3	1:A:521:ILE:HD11	2.01	0.42
1:A:167:LYS:CG	1:A:718:THR:HG23	2.50	0.42
1:A:503:PHE:HB2	1:A:532:VAL:HG12	2.02	0.42
1:A:677:ARG:CB	1:A:677:ARG:HH11	2.32	0.42
1:A:73:THR:HG23	1:A:74:PRO:HD2	2.01	0.42
1:A:451:TRP:O	1:A:452:ASP:O	2.38	0.42
1:A:239:PRO:O	1:A:276:SER:HB3	2.20	0.42
6:A:904:LIL:H9F1	8:A:906:LIM:C5X	2.48	0.42
1:A:529:GLN:HA	1:A:551:ASN:O	2.20	0.42
1:A:390:TRP:CH2	1:A:431:PRO:HG3	2.55	0.42
1:A:317:VAL:HA	1:A:340:TYR:O	2.20	0.42
1:A:495:PHE:HB3	1:A:496:ASP:H	1.49	0.41
1:A:74:PRO:HB2	1:A:580:GLU:HB3	2.02	0.41
1:A:453:LYS:HA	1:A:453:LYS:HE2	2.02	0.41
1:A:127:GLU:O	1:A:128:ARG:HB3	2.20	0.41
6:A:903:LIL:C8E	6:A:904:LIL:H0S1	2.50	0.41
1:A:494:LEU:HA	1:A:500:THR:HG23	2.02	0.41
1:A:122:ASP:O	1:A:125:MET:HG2	2.21	0.41
1:A:471:ASN:O	1:A:475:GLY:N	2.54	0.41
1:A:495:PHE:HD2	1:A:497:ASN:OD1	2.04	0.41
1:A:312:VAL:HG11	1:A:343:ARG:HH21	1.86	0.41
1:A:563:GLU:O	1:A:564:GLY:O	2.38	0.41
1:A:199:ARG:HG2	1:A:200:SER:N	2.36	0.41
6:A:903:LIL:H2E2	6:A:904:LIL:H4E2	2.03	0.40
6:A:903:LIL:H3E1	6:A:903:LIL:H2F2	1.85	0.40
1:A:56:GLU:H	1:A:56:GLU:CD	2.24	0.40
1:A:33:SER:OG	1:A:34:ALA:N	2.54	0.40
1:A:300:LEU:HD12	1:A:357:VAL:HG13	2.02	0.40
1:A:611:LYS:C	1:A:613:ASN:H	2.24	0.40
1:A:74:PRO:HA	10:A:1082:HOH:O	2.21	0.40
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.56	0.40
1:A:352:LEU:HD12	1:A:352:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1002:KDO:H7	2:A:1004:GMH:C1	2.51	0.40
1:A:581:ILE:HG12	1:A:597:TYR:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	703/723 (97%)	633 (90%)	57 (8%)	13 (2%)	11 18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	452	ASP
1	A	564	GLY
1	A	634	GLY
1	A	418	ASP
1	A	611	LYS
1	A	680	MET
1	A	495	PHE
1	A	674	ASP
1	A	398	PRO
1	A	334	PRO
1	A	368	GLY
1	A	405	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	585/599 (98%)	563 (96%)	22 (4%)	40 67

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	76	VAL
1	A	93	ARG
1	A	101	SER
1	A	112	GLN
1	A	118	ASP
1	A	128	ARG
1	A	132	MET
1	A	144	SER
1	A	148	LEU
1	A	205	GLN
1	A	275	TYR
1	A	352	LEU
1	A	353	GLN
1	A	354	ASN
1	A	357	VAL
1	A	397	VAL
1	A	404	ASN
1	A	428	ASN
1	A	453	LYS
1	A	496	ASP
1	A	720	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	165	GLN
1	A	202	ASN
1	A	205	GLN
1	A	288	HIS
1	A	310	ASN
1	A	328	GLN

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Mol	Chain	Res	Type
1	A	353	GLN
1	A	354	ASN
1	A	388	ASN
1	A	410	HIS
1	A	412	HIS
1	A	416	ASN
1	A	428	ASN
1	A	520	ASN
1	A	551	ASN
1	A	688	HIS
1	A	690	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KDO	A	1002	2	12,15,16	0.78	0	12,21,24	0.78	0
2	KDO	A	1003	2	12,15,16	0.50	0	12,21,24	0.61	0
2	GMH	A	1004	9,2	13,13,14	1.48	3 (23%)	17,18,20	1.40	4 (23%)
3	GLC	A	1006	3	11,11,12	0.75	0	14,15,17	1.20	2 (14%)
3	GLA	A	1007	3	11,11,12	0.61	0	14,15,17	0.89	1 (7%)
3	GLA	A	1009	3	11,11,12	0.47	0	14,15,17	0.84	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GP4	A	901	2,6	15,15,16	1.14	1 (6%)	18,22,24	1.87	3 (16%)
2	GP1	A	902	8,2,4,7	15,16,16	1.28	2 (13%)	20,24,24	0.90	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KDO	A	1002	2	-	0/6/26/30	0/1/1/1
2	KDO	A	1003	2	-	0/6/26/30	0/1/1/1
2	GMH	A	1004	9,2	-	0/6/23/26	0/1/1/1
3	GLC	A	1006	3	-	0/2/19/22	0/1/1/1
3	GLA	A	1007	3	-	0/2/19/22	0/1/1/1
3	GLA	A	1009	3	-	0/2/19/22	0/1/1/1
2	GP4	A	901	2,6	-	0/7/24/27	0/1/1/1
2	GP1	A	902	8,2,4,7	-	0/6/27/27	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	GP4	P4A-O4A	-3.21	1.50	1.60
2	A	902	GP1	P4B-O1B	-2.93	1.51	1.60
2	A	1004	GMH	O3-C3	2.06	1.47	1.43
2	A	1004	GMH	C1-C2	2.29	1.57	1.52
2	A	902	GP1	C3B-C2B	2.71	1.57	1.53
2	A	1004	GMH	C2-C3	3.48	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	GP4	P4A-O4A-C4A	-3.91	112.19	121.56
3	A	1006	GLC	C2-C3-C4	-2.03	107.59	111.04
2	A	902	GP1	C3B-C2B-N2B	2.03	114.62	110.86
2	A	1004	GMH	C1-C2-C3	2.12	112.05	109.54
2	A	1004	GMH	C3-C4-C5	2.49	115.07	109.60
2	A	1004	GMH	O5-C5-C6	2.56	109.46	106.04
3	A	1007	GLA	C1-O5-C5	2.66	115.62	112.25
3	A	1006	GLC	C1-O5-C5	2.69	115.66	112.25
2	A	1004	GMH	O3-C3-C2	2.71	114.89	110.00
3	A	1009	GLA	C1-O5-C5	2.84	115.86	112.25
2	A	901	GP4	C1A-O6A-C5A	3.22	116.34	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	GP4	C1A-C2A-C3A	5.29	117.83	109.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	KDO	1	0
2	A	1004	GMH	2	0
3	A	1006	GLC	6	0
3	A	1009	GLA	6	0
2	A	902	GP1	1	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GPO	A	1005	4	17,17,18	1.43	2 (11%)	22,25,27	1.59	3 (13%)
9	EA2	A	1008	2	5,10,11	1.20	0	6,13,16	1.12	0
6	LIL	A	903	2	30,30,31	0.72	1 (3%)	30,31,33	0.99	1 (3%)
6	LIL	A	904	2	30,30,31	0.66	1 (3%)	30,31,33	0.97	1 (3%)
7	AAE	A	905	2	5,5,6	3.20	2 (40%)	3,5,7	2.99	2 (66%)
8	LIM	A	906	2	16,16,17	3.02	1 (6%)	13,16,18	2.18	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GPO	A	1005	4	-	0/11/28/31	0/1/1/1
9	EA2	A	1008	2	-	0/8/10/11	0/0/0/0
6	LIL	A	903	2	-	2/31/31/32	0/0/0/0
6	LIL	A	904	2	1/1/2/3	0/31/31/32	0/0/0/0
7	AAE	A	905	2	-	0/2/3/4	0/0/0/0
8	LIM	A	906	2	-	0/14/15/16	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	GPO	P-O4	-3.27	1.50	1.60
7	A	905	AAE	C4-C5	2.76	1.55	1.52
5	A	1005	GPO	C2-C3	2.81	1.56	1.52
6	A	904	LIL	O2E-C1F	3.19	1.43	1.34
6	A	903	LIL	O2E-C1F	3.59	1.45	1.34
7	A	905	AAE	O8-C5	6.38	1.44	1.21
8	A	906	LIM	O2J-C3J	11.99	1.43	1.21

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	906	LIM	O2J-C3J-C2J	-6.72	109.36	120.82
7	A	905	AAE	O8-C5-C9	-4.47	110.27	121.31
6	A	903	LIL	O2E-C1F-O1F	-3.90	113.21	123.67
5	A	1005	GPO	P-O4-C4	-3.82	112.41	121.56
6	A	904	LIL	O2E-C1F-O1F	-3.66	113.85	123.67
8	A	906	LIM	O2J-C3J-C4J	-3.57	109.86	121.16
7	A	905	AAE	O8-C5-C4	-2.35	111.35	120.96
5	A	1005	GPO	C1-C2-C3	2.27	112.22	109.54
5	A	1005	GPO	O5-C5-C6	2.91	109.93	106.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	904	LIL	C3E

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	903	LIL	C3E-O2E-C1F-C2F
6	A	903	LIL	C3E-O2E-C1F-O1F

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1008	EA2	1	0
6	A	903	LIL	11	0
6	A	904	LIL	7	0
7	A	905	AAE	1	0
8	A	906	LIM	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	705/723 (97%)	-0.07	14 (1%) 68 72	35, 64, 99, 119	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	LYS	4.3
1	A	723	PHE	3.8
1	A	19	GLU	3.7
1	A	635	PRO	3.2
1	A	519	GLY	2.8
1	A	566	PHE	2.7
1	A	632	PHE	2.6
1	A	119	ALA	2.5
1	A	99	GLY	2.5
1	A	366	ALA	2.5
1	A	101	SER	2.1
1	A	369	ASP	2.1
1	A	121	ILE	2.1
1	A	332	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GP4	A	901	15/16	0.96	0.13	-1.95	35,53,71,81	0
2	KDO	A	1002	15/16	0.98	0.11	-2.33	49,60,76,92	0
3	GLA	A	1009	11/12	0.88	0.31	-	101,111,120,120	0
2	GMH	A	1004	13/14	0.96	0.12	-	44,58,75,81	0
2	KDO	A	1003	15/16	0.91	0.20	-	69,78,84,87	0
3	GLA	A	1007	11/12	0.89	0.32	-	97,110,116,117	0
3	GLC	A	1006	11/12	0.92	0.31	-	80,98,107,114	0
2	GP1	A	902	16/16	0.96	0.10	-	53,65,80,83	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	LIL	A	903	31/32	0.90	0.27	6.34	65,82,92,95	0
8	LIM	A	906	17/18	0.95	0.21	3.27	57,69,86,97	0
6	LIL	A	904	31/32	0.95	0.18	1.13	46,65,74,84	0
9	EA2	A	1008	11/12	0.94	0.15	-	59,102,120,120	0
4	NI	A	1011	1/1	0.90	0.05	-	100,100,100,100	0
4	NI	A	1012	1/1	0.84	0.11	-	120,120,120,120	0
7	AAE	A	905	6/7	0.82	0.24	-	82,95,101,105	0
5	GPO	A	1005	17/18	0.87	0.18	-	52,84,106,113	0

6.5 Other polymers (i)

There are no such residues in this entry.